**UNIVERSITY OF ABERDEEN SCHOOL OF ENGINEERING**

**COURSE INFORMATION SESSION 2018/19**

**EG2XXX Introduction to Chemical Engineering**

**CREDIT POINTS:**

15

**COURSE CO-ORDINATOR:**

TBC

**COURSE ORGANISER:**

TBC

**CONTRIBUTORS:**

TBC

**SCRUTINEER:**

TBC

**PRE-REQUISITE:**

**CO-REQUISITE:**

None

**COURSES FOR WHICH THIS COURSE IS A PRE-REQUISITE:**

None

**AIMS**

The course aims to provide understanding of main principles and techniques underpinning material and energy balances in chemical engineering processes combining numerical methods with practical experience using appropriate software. The course develops a foundation for understanding, developing and analysing successful simulations of fluid flows applicable to a broad range of applications.

**DESCRIPTION**

Topics: overall staged separations, material and energy balances, concepts of rate processes, energy and mass transport, and kinetics of chemical reactions. Applications of these concepts to areas of current technological importance: biotechnology, energy, production of chemicals, materials processing, and purification.

The course will provide insight into physical phenomena in environmental and industrial fluid flows via numerical simulations. Whist this motivates the use of computational technologies, even advanced CFD software may lead to incorrect predictions of fluid flow behaviour if used without sufficient understanding of the underlying algorithms and methods. This course introduces students to computational methods for solving distinct type of partial differential equations (PDE) that arise in fluid dynamic studies.

This course will involve fundamentals of numerical analysis of PDE, introduction to computational linear algebra, discretisation techniques and numerical schemes to solve time-dependent PDE problems, error control and stability analysis, mesh-generation methods and turbulence models. Hands-on sessions with industry standard software are used to develop CFD skills.

**LEARNING OUTCOMES**

By the end of the course students should:

**A: have knowledge and understanding of:**

* Fundamental computational fluid dynamics and applications;
* Finite difference and finite volume discretisation of PDE's and how numerical techniques are applied to flow equations;
* CFD workflow procedures including mesh generation, numerical discretisation schemes and solver methods, assignment of appropriate initial and boundary conditions, pre- and post-processing data.

**B: have gained intellectual skills so that they are able to:**

* Select appropriate set of numerical methods and discretisation schemes for a particular fluid flow application;
* Recognise terminologies used by CFD practitioners (e.g., mesh grid, boundary conditions, numerical schemes, linear solvers, quality assurance, HPC etc);
* Assess the applicability of a particular model/method and its limitations;
* Choose appropriate type of boundary conditions and mesh-grid types for simulations and assess grid dependence;
* Set up simple CFD problems;
* Analyse and interpret data obtained from the numerical simulations.

**C: have gained practical skills so that they are able to:**

* Use programming languages to numerically solve 1- and 2-D time-dependent PDE's (e.g., advection-diffusion equations);
* Use commercial CFD software to simulate fluid flow regimes relevant to engineering applications.

**D: have gained or improved transferable skills so that they are able to:**

* Use commercial CFD software to build flow geometries, generate adequate mesh grid for an accurate solution, select appropriate solvers to obtain a flow solution and visualise the simulated data;
* Use computational tools and programming languages to support data processing and manipulation;
* Perform critical analysis on data resulting from CFD simulations.

**SYLLABUS**

**Module 1** Introduction to Chemical Engineering Calculations: (3 lectures)

1. Units and dimensions;
2. Conversion of units;
3. Dimensional homogeneity and dimensionless quantities;
4. Mole and molecular weight;
5. Process and process variables;
6. Process classification: batch process, continuous process, and semibatch process, steady-state and transient.

**Module 2** Fundamentals of Material Balances: (7 lectures)

1. Introduction to mass conservation equation;
2. Material balance calculation practices;
3. Mass balance in non-reactive systems;
4. Recycle and by-pass;
5. Mass balance in reactive systems;
6. Chemical reaction definitions: limiting reactant, excess reactant, conversion rate and selectivity;
7. Chemical reaction stoichiometry;
8. Molecular species balances;
9. Material balance in combustion reactions;
10. Material balance in multiphase systems.

**Module 3** Fundamentals of Energy Balance: (6 lectures)

1. Internal, kinetic and potential energy;
2. Work, heat and enthalpy;
3. First and second laws of thermodynamics applied to closed and open systems;
4. Energy balance calculation practices;
5. Energy balance in non-reactive systems;
6. Processes with no phase change: sensible heat;
7. Processes with phase change: latent heat;
8. Heat of reaction, formation and combustion.

**Module 4** Combined Material and Energy Balance: (5 lectures)

1. Gibbs phase rule: degrees of freedom analysis;
2. Raoult’s law and flash calculations;
3. Case studies of industrial processes and unit operations (distillation, cristalisation, etc) involving:
   1. Production of organic compounds;
   2. Bioengineering process.

**Module 5** Computer-Aided Balance Calculations (hands-on sessions): (12 lectures)

1. Gibbs phase rule: degrees of freedom analysis;
2. Introduction to programming languages;
3. Basic elements of programming in Matlab;
4. Case-studies of combined material and energy conservation analysis with Matlab;
5. Introduction to ASPEN process simulator;
6. Case-studies of combined material and energy conservation analysis with ASPEN.

**TIMETABLE**

Lectures: 3 one-hour per week (over 7 weeks);

Practicals: 1 three-hours per week (over 4 weeks);

Tutorials: 1 one-hour per week.

Total Hours: 100 ( Lecture Hours 11, Supervised Practical/Workshop/Studio Hours 33, Formative Assessment Hours 1, Summative Assessment Hours 6, Programme Level Learning and Teaching Hours 2, Directed Learning and Independent Learning Hours 47 )

**ASSESSMENT**

**1st attempt:** 1 three-hour written examination paper (60%) and continuous assessment (40%).

**Resit:** A three-hour resit paper will be provided for candidates who fail the course at the first attempt.

The continuous assessment (CA) will consist of 2 components:

* Problem solving programming exercises (50%);
* Individual report on assigned Engineering problem with ASPEN process simulator (50%).

These activities will be based on the submission of reports detailing assigned computational work. Detailed information relating to the format of reports will be given during course contact time.

**Notes on Assessment:**

* Students are required to pass both the examination and the continuous assessment in order to pass the course. A fail in the exam will not be condoned by a pass in other elements of assessment;
* In the case of a fail in any element of assessment the overall course grade will be limited to E1;
* Candidates who fail the written examination at the first attempt will be required to pass the *resit* examination;
* Candidates who pass the examination at the first attempt but fail to pass the CA elements will be required to pass the *resit* of the failed CA component(s);
* **Penalties** for late or non-submission of in-course work are defined in the Undergraduate Student Handbook which is available on the *MyAberdeen* pages for each course. If you are absent on medical grounds or other good cause, the University's policy on requiring a medical or self-certificate can be found at:

[www.abdn.ac.uk/staffnet/teaching/aqh/appendix7x5.pdf](http://www.abdn.ac.uk/staffnet/teaching/aqh/appendix7x5.pdf)

You are strongly advised to make yourself fully aware of your responsibilities if absent due to illness or other good cause. In particular, you are asked to note when self-certification of absence is permitted or if you are required to submit a medical certificate. All absences (medical or otherwise) should be reported through *MyAberdeen*, where you can access a student absence form for completion. *MyAberdeen* will allow you to upload any required supporting documentation, such as a medical certificate.

**FORMAT OF EXAMINATION**

Candidates must attempt **ALL FOUR** questions. All questions carry 25 marks. Notes:

* Candidates are permitted to use approved calculators only;
* Candidates are permitted to use the Engineering Mathematics Handbook, which will be made available to them.

**FEEDBACK**

* Students can receive feedback on their progress with the Course on request at the weekly tutorial/feedback sessions;
* Students are given feedback through formal marking and return of practical reports;
* Students requesting feedback on their exam performance should make an appointment within 2 weeks of the publication of the exam results.

**RECOMMENDED BOOKS**

1. J.H. Fereziger and M. Peric, *Computational Methods for Fluid Dynamics*, 2001;
2. H. Versteeg and W. Malalasekra, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*, 2007;
3. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Numerical Recipes: The Art of Scientific Computing*, 2007;
4. J. Kiusalaas, *Numerical Methods in Engineering with Python*, 2014;
5. J. Kiusalaas, *Numerical Methods in Engineering with Matlab*, 2009;
6. O.C. Zienkiewicz and R.L. Taylor, *The Finite Element Method -- Fluid Dynamics (Vol 3)*, 2004;
7. G.H. Golub and C.F. Van Loan, *Matrix Computations*, 1996;
8. C. Hirsh, *Numerical Computation of Internal and External Flows (Vols 1 and 2)*, 2002.

**INSTITUTIONAL INFORMATION**

Students are asked to make themselves familiar with the information on key institutional policies which have been made available within *MyAberdeen*,

<https://abdn.blackboard.com/bbcswebdav/institution/Policies>

These policies are relevant to all students and will be useful to you throughout your studies. They contain important information and address issues such as what to do if you are absent, how to raise an appeal or a complaint and how seriously the University takes your feedback.

These institutional policies should be read in conjunction with this programme and/or course handbook, in which School and College specific policies are detailed. Further information can be found on the [University's Infohub webpage](http://www.abdn.ac.uk/infohub/) or by visiting the *Infohub*.